

10/502,032

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	536	(556/12).CCLS.	US-PGPUB; USPAT; EPO; JPO	OR	OFF	2006/08/21 16:50
L2	588	(556/28).CCLS.	US-PGPUB; USPAT; EPO; JPO	OR	OFF	2006/08/21 16:56
L3	2060	(502/152).CCLS.	US-PGPUB; USPAT; EPO; JPO	OR	OFF	2006/08/21 17:14
L4	2413	(526/160).CCLS.	US-PGPUB; USPAT; EPO; JPO	OR	OFF	2006/08/21 17:14

10/502,073

(FILE 'HOME' ENTERED AT 11:14:08 ON 21 AUG 2006)

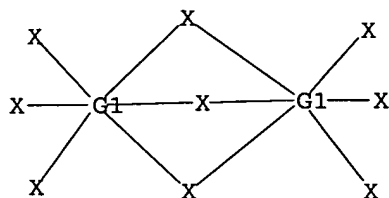
FILE 'REGISTRY' ENTERED AT 11:14:22 ON 21 AUG 2006

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 Hf,Zr

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:14:55 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 133 TO ITERATE

100.0% PROCESSED 133 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1969 TO 3351

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 11:15:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3075 TO ITERATE

100.0% PROCESSED 3075 ITERATIONS

49 ANSWERS

SEARCH TIME: 00.00.01

L3 49 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'CAPLUS' ENTERED AT 11:15:05 ON 21 AUG 2006

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FILE LAST UPDATED: 20 Aug 2006 (20060820/ED)

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<http://www.cas.org/infopolicy.html>

=> s 13

L4 41 L3

=> d 1-41 bib abs

L4 ANSWER 1 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:334107 CAPLUS

DN 145:90451

TI Periodic trends in metal-metal interactions in face-shared [M2Cl9]z- systems

AU Cavigliasso, German; Lovell, Timothy; Stranger, Robert

CS Department of Chemistry, Faculty of Science, Australian National University, Canberra, 0200, Australia

SO Dalton Transactions (2006), (16), 2017-2025

CODEN: DTARAF; ISSN: 1477-9226

PB Royal Society of Chemistry

DT Journal

LA English

AB The periodic trends in metal-metal interactions in even-electron and mixed-valence [M2Cl9]z- face-shared systems, involving transition metals in Groups 4 to 8 and electronic configurations ranging from d1d1 through to d5d5 and from d1d2 through to d4d5, have been investigated by calculating metal-metal bonding and spin polarization (exchange) effects using d. functional theory. These two terms are in opposition to one another and their relative difference det. the extent to which the metal-based electrons are delocalized and thus the degree of metal-metal bonding. Remarkably strong linear correlations between the two terms, and between each term and the square of the spin d. on the metal centers, have been obtained for all group and period series considered, and are discussed in terms of their dependence on the metal orbital properties and electron d.

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:500061 CAPLUS

DN 143:451587

TI Thermal behavior of ammonium-bearing zirconium and hafnium fluoro complexes with hydrofluoride

AU Antokhina, T. F.; Savchenko, N. N.; Merkulova, E. B.; Kaidalova, T. A.; Polishchuk, S. A.

CS Inst. Khim., DVO RAN, Vladivostok, Russia

SO Zhurnal Neorganicheskoi Khimii (2005), 50(4), 707-709

CODEN: ZNOKAQ; ISSN: 0044-457X

PB MAIK Nauka/Interperiodica Publishing

DT Journal

LA Russian

AB (NH4)4MA3F17.2HF (M = Li, Na; A = Zr, Hf) were studied by DTA and x-ray phase anal. At 120-230Å dehydrofluorination of (NH4)4MA3F17.2HF occurred, leading to decomposition and the formation of ammonium and sodium/lithium containing fluoro complexes.

L4 ANSWER 3 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:376673 CAPLUS
DN 143:317823
TI Chemical properties of $(\text{NH}_4)_2\text{SiF}_6$
AU Mel'nichenko, E. I.; Krysenko, G. F.; Epov, D. G.
CS Inst. Khim., DVO RAN, Vladivostok, Russia
SO Zhurnal Neorganicheskoi Khimii (2005), 50(2), 192-196
CODEN: ZNOKAQ; ISSN: 0044-457X
PB MAIK Nauka/Interperiodica Publishing
DT Journal
LA Russian
AB The solid phase reaction of $(\text{NH}_4)_2\text{SiF}_6$ with SiO_2 led to the formation of SiF_4 , NH_3 , NH_4SiF_5 , and H_2O . The reaction with CaCO_3 and CaO led to the decomposition of SiF_6^{2-} to SiO_2 . The solid phase reaction of $(\text{NH}_4)_2\text{SiF}_6$ with various metal fluorides led to the formation of $\alpha\text{-NH}_4\text{ZrF}_5$ and $\text{NH}_4\text{Zr}_2\text{F}_9$ with ZrF_4 and $(\text{NH}_4)_3\text{AlF}_6$ which decomposed to NH_4AlF_4 from AlF_3 .

L4 ANSWER 4 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:309278 CAPLUS
DN 143:393338
TI Quantum-chemical study of potassium and ammonium hexafluorozirconates
AU Voit, E. I.; Voit, A. V.; Kavun, V. Ya.; Sergienko, V. I.
CS Institute of Chemistry, Far East Branch, Russian Academy of Sciences, Vladivostok, Russia
SO Journal of Structural Chemistry (2004), 45(4), 610-616
CODEN: JSTCAM; ISSN: 0022-4766
PB Springer Science+Business Media, Inc.
DT Journal
LA English
AB A number of fluorozirconate clusters serving as structural models for K_2ZrF_6 and $(\text{NH}_4)_2\text{ZrF}_6$ crystals were investigated by the Hartree-Fock ab initio method. Based on the results of quantum-chemical calcns. it is shown that the differences in the structure of these compds. and in the behavior of the temperature dependence of the second moment of the ^{19}F NMR spectra are due to differences in the binding between the cation and anion sublattices. A mechanism responsible for ionic mobility is suggested.
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:205155 CAPLUS
DN 142:430407
TI Reactivity of Silyl-Substituted Allyl Compounds with Group 4, 5, 9, and 10 Metals: Routes to η^3 -Allyls, Alkylidenes, and sec-Alkyl Carbocations
AU Schormann, Mark; Garratt, Shaun; Bochmann, Manfred
CS Wolfson Materials and Catalysis Centre, School of Chemical Sciences, University of East Anglia, Norwich, NR4 7TJ, UK
SO Organometallics (2005), 24(7), 1718-1724
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
OS CASREACT 142:430407
AB Whereas the reaction of alkali-metal salts of silyl-allyls $\text{E}^+[\text{C}_3\text{H}_3(\text{SiMe}_3)_2\text{-1,3}]^-$ ($\text{E} = \text{Li}, \text{K}$) with Group 4 and Group 5 metal halides gave intractable reduction products, $\text{Co}(\text{acac})_3$ and $\text{Ni}(\text{acac})_2$ reacted with $\text{K}[\text{C}_3\text{H}_3(\text{SiMe}_3)_2\text{-1,3}]$ to give $\text{Co}\{\eta^3\text{-C}_3\text{H}_3(\text{SiMe}_3)_2\text{-1,3}\}_2$ (1) and $\text{Ni}\{\eta^3\text{-C}_3\text{H}_3(\text{SiMe}_3)_2\text{-1,3}\}_2$ (2), resp. The reaction of $\text{K}[\text{C}_3\text{H}_3(\text{SiMe}_3)_2\text{-1,3}]$ with Me_3SnCl afforded $\text{Me}_3\text{SiCH:CHCH}(\text{SiMe}_3)(\text{SnMe}_3)$ (3), which reacted cleanly with TaCl_5 to give $\{\eta^3\text{-C}_3\text{H}_3(\text{SiMe}_3)_2\text{-1,3}\}\text{TaCl}_4$ (4). Treatment of this complex with tetramethylethylenediamine led to HCl abstraction, and the allyl complex was transformed into the vinyl-alkylidene compound $\text{Me}_3\text{SiCH:CHC}(\text{SiMe}_3):\text{TaCl}_3(\text{TMEDA})$ (5). Whereas in the case of TaCl_5 dehalostannylation was facile, the reaction of 3 with ZrCl_4 and HfCl_4 took a different course, leading instead to the addition of

Me₃Sn⁺ to 3 to give [HC{CH(SiMe₃)(SnMe₃)}₂]+[M₂Cl₉]⁻ (6, M = Zr; 7, M = Hf), the first examples of isolable sec-alkyl carbocations. These salts are surprisingly thermally stable and melt >100 °C; this stability is largely due to delocalization of the pos. charge over the two tin atoms. The crystal structures of 1, 2, and 5-7 are reported.

RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:591223 CAPLUS
DN 139:150077
TI Process for preparing isobutylene-based polymers
IN Bochmann, Manfred; Garratt, Shaun; Schormann, Mark
PA Bayer Inc., Can.
SO PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003062284	A2	20030731	WO 2003-CA67	20030121
	WO 2003062284	A3	20031002		
	WO 2003062284	C1	20031204		
	W:		AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW		
	RW:		GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG		
	CA 2368724	AA	20030721	CA 2002-2368724	20020121
	EP 1470167	A2	20041027	EP 2003-700268	20030121
	R:		AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK		
	CN 1620470	A	20050525	CN 2003-802539	20030121
	JP 2005515276	T2	20050526	JP 2003-562161	20030121
	US 2005165182	A1	20050728	US 2003-502073	20030121
PRAI	CA 2002-2368724	A	20020121		
	WO 2003-CA67	W	20030121		

OS MARPAT 139:150077
AB This invention relates to a metal organic compound, a catalytic composition comprising said metal organic compound, a process for homo- or co-polymerizing isoolefines in the presence of said metal organic compound and a method of stabilizing a compound of the general structure [R'HC(CRR')₂]₂+ [M₂X₉]⁻, in which R = SiR₁R₂R₃, R' = hydrogen, C₁-12 alkyl, C₆-14 aryl, or C₇-20 alkylaryl, M = Zr or Hf, X = halogen, and R₁-3 C₁-12 alkyl group, with a compound R' = the formula M'R₄R₅R₆, in which M' = Si, Ge, Sn, or Pb and R₄-6 = C₁-12 alkyl group as well as a non-coordinating anion of the general structure [M₂X₉]⁻ in which M = Zr or Hf and X = halogen atom.

L4 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:42082 CAPLUS
DN 138:95272
TI Composition for oral hygiene comprising a fluoride ion vector and an antioxidant
IN Cazor, Jean-Louis; Lhuisset, Francois; Robineau, Pascale
PA Sanofi-Synthelabo, Fr.
SO PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DT Patent

LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003003995	A1	20030116	WO 2002-FR2313	20020703
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	FR 2826868	A1	20030110	FR 2001-8852	20010704
	EP 1408921	A1	20040421	EP 2002-782462	20020703
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	JP 2004535453	T2	20041125	JP 2003-510007	20020703
	US 2004258634	A1	20041223	US 2004-481718	20040722
PRAI	FR 2001-8852	A	20010704		
	WO 2002-FR2313	W	20020703		

AB The invention concerns a composition for oral hygiene adapted for diabetics. The inventive composition comprises at least a fluoride ion vector and at least an antioxidant and can in particular be in the form of a toothpaste, a chewing gum, a mouthwash, a spray. The invention also concerns the use of at least a fluoride ion vector and at least an antioxidant for preparing a composition for oral hygiene designed to prevent and/or fight against oral pathologies in diabetics.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:655583 CAPLUS
DN 137:337966
TI Isolation and Structure of $[HC\{CH(SiMe_3)(SnMe_3)\}_2]^+$: A Remarkably Stable sec-Alkyl Cation
AU Schormann, Mark; Garratt, Shaun; Hughes, David L.; Green, Jennifer C.; Bochmann, Manfred
CS Wolfson Materials and Catalysis Centre, School of Chemical Sciences, University of East Anglia, Norwich, NR4 7TJ, UK
SO Journal of the American Chemical Society (2002), 124(38), 11266-11267
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 137:337966

AB The reaction of the tin-substituted propene $Me_3Sn(R)CHCH:CHR$ ($R = SiMe_3$) with MCl_4 in dichloromethane in the presence of Me_3SnCl gives the first examples of isolable sec-alkyl carbocation salts, $[HC(CH(R)SnMe_3)_2]^+M_2Cl_9^-$ ($M = Zr, Hf$). The compds. are thermally stable and, unlike previously isolated trialkyl carbocations, do not require superacidic media or weakly coordinating anions for stability. The crystal structure and DFT calcns. suggest polarization of the Sn substituents and hyperconjugation as the reason for the unexpected stability. The stabilizing effect of tin is significantly stronger than that of Si. The carbocations are effective initiators for the polymerization of isobutene, isoprene, and α -methylstyrene.

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:591718 CAPLUS
 DN 133:313907
 TI Quantum chemical study of model fluorozirconate clusters
 AU Voit, E. I.; Voit, A. V.; Gerasimenko, A. V.; Sergienko, V. I.
 CS Institute of Chemistry, Far East Branch, Russian Academy of Sciences,
 Vladivostok, Russia
 SO Journal of Structural Chemistry (Translation of Zhurnal Strukturnoi
 Khimii) (2000), 41(1), 41-47
 CODEN: JSTCAM; ISSN: 0022-4766
 PB Consultants Bureau
 DT Journal
 LA English
 AB Fluorozirconate clusters [Zr_mF_n](4m-n) were investigated by the
 DV-X α quantum chemical method and the results were used to explain the
 existence of polyhedra with central-atom coordination nos. 6, 7, and 8 in
 crystalline fluorozirconates. The [ZrF₆]²⁻ octahedron and the dimer of
 edge-sharing seven-vertex polyhedra [Zr₂F₁₂]⁴⁻ are highly stable.
 RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2000:171560 CAPLUS
 DN 132:326211
 TI Coordination polyhedrons HfX_n (X = halogen) in the structures of Hf(IV)
 compounds
 AU Serezhkina, L. B.; Serezhkin, V. N.; Davidovich, R. L.
 CS Samara State University, Samara, Russia
 SO Russian Journal of Coordination Chemistry (Translation of
 Koordinatsionnaya Khimiya) (2000), 26(1), 18-22
 CODEN: RJCCEY; ISSN: 1070-3284
 PB MAIK Nauka/Interperiodica Publishing
 DT Journal
 LA English
 AB The Voronoi-Dirichlet polyhedrons and the method of intersecting spheres
 were used to carry out crystallochem. anal. of all the structurally
 studied compds. containing coordination polyhedrons HfX_n (X = F, Cl, and I).
 The Hf(IV) coordination number (C.N.) is shown to be 6, 7, or 8 with respect
 to the F atoms and only 6 with respect to the Cl or I atoms. It is
 established that, although the Hf-X distances in HfX_n vary by more than
 0.3 Å, the volume of the Voronoi-Dirichlet polyhedron of the Hf(IV) atom
 virtually does not depend on the metal C.N. (for X = F) or on the degree
 of distortion of the HfX₆ octahedron (for X = Cl and I).
 RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1999:722907 CAPLUS
 DN 131:327376
 TI Use of a fluoride ion vector for preparing a medicine for preventing or
 treating diseases associated with Helicobacter pylori
 IN Finidori, Claudine
 PA Sanofi-Synthelabo, Fr.
 SO PCT Int. Appl., 16 pp.
 CODEN: PIXXD2
 DT Patent
 LA French
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9956756	A1	19991111	WO 1999-FR920	19990420
	W:				
	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,				
	DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,				
	JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK,				
	MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,				

TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

FR 2778104	A1	19991105	FR 1998-5597	19980504
FR 2778104	B1	20020830		
AU 9933364	A1	19991123	AU 1999-33364	19990420
EP 1075268	A1	20010214	EP 1999-914615	19990420
EP 1075268	B1	20050727		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

AT 300307	E	20050815	AT 1999-914615	19990420
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PRAI FR 1998-5597 A 19980504
WO 1999-FR920 W 19990420

AB The use of at least one pharmaceutically acceptable fluoride ion vector for preparing a medicine for prevention or adjuvant therapy treatment of a disease associated with *Helicobacter pylori* is disclosed. A dentifrice contained sodium fluoride 0.33, sodium monofluorophosphate 0.76, silica 21.00, carrageenan 11.00, titanium oxide 1.00, phosphates 0.30, sodium benzoate 4.00, sorbitol 25.00, preservatives 0.10, fragrances 1.06, and water q.s. 100.00%.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:756569 CAPLUS
DN 130:115327
TI Metal-Metal Bonding in d1d1 and d2d2 Biocuboctahedral Dimer Systems: A Density Functional Study of Face-Shared M₂X₉- (M = Ti, Zr, Hf, V, Nb, Ta) Complexes
AU Stranger, Robert; McGrady, John E.; Lovell, Timothy
CS Department of Chemistry, The Faculties, The Australian National University, Canberra, 0200, Australia
SO Inorganic Chemistry (1998), 37(26), 6795-6806
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
AB D. functional theory is used to investigate the electronic and geometric structures and periodic trends in metal-metal bonding of d1d1 and d2d2 face-shared M₂X₉- dimers of Ti, Zr, Hf (d1d1) and V, Nb, Ta (d2d2). For these systems three distinct coupling modes can be recognized, depending on the occupation of the trigonal t_{2g}(a₁ + e) single-ion orbitals, which determine the ground-state geometry and extent of metal-metal bonding. For Ti₂Cl₉-, the [a₁ + a₁] broken-symmetry optimized structure, corresponding to significant delocalization of the metal-based σ electrons, nicely rationalizes the strong antiferromagnetic coupling reported for Cs₃Ti₂Cl₉. The ground-state geometries for Zr₂Cl₉- and Hf₂Cl₉- correspond to complete delocalization of the metal-based electrons in a metal-metal σ bond. For V₂Cl₉-, the global min. is found to be the ferromagnetic [a₁e + e₂] spin-quintet state giving rise to a long V-V separation, consistent with the known structure and reported weak ferromagnetic behavior of Cs₃V₂Cl₉. For Nb₂X₉- (X = Cl, Br, I) and Ta₂Cl₉-, the [a₁e + a₁e] spin-triplet state, where complete delocalization of the σ and δπ electrons occur in a metal-metal double bond, is found to be the global min. and consequently relatively short internuclear distances result, again, in good agreement with experiment. The periodic trends in metal-metal bonding in these and the isovalent d3d3 complexes can be rationalized in terms of the energetic contributions of orbital overlap (ΔE_{ovlp}) and spin polarization (ΔE_{spe}), the difference ΔE_{spe} - ΔE_{ovlp} determining the tendency of the metal-based electrons to delocalize in the dimer. For d1d1 systems, ΔE_{ovlp} is always greater than ΔE_{spe} and

therefore delocalized ground states result for all complexes of the titanium triad. Across the first transition series, the dramatic increase in ΔE_{spe} dominates ΔE_{ovlp} and therefore $\text{V}_2\text{Cl}_{19}^-$ and $\text{Cr}_2\text{Cl}_{19}^-$ have localized ground states. For the second and third transition series, the much larger ΔE_{ovlp} term ensures that all these complexes remain delocalized.

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:135171 CAPLUS
DN 128:236521
TI Vibrational modes and structure of liquid and gaseous zirconium tetrachloride and of molten ZrCl_4 - CsCl mixtures
AU Photiadis, G. M.; Papatheodorou, G. N.
CS Department of Chemical Engineering, Institute of Chemical Engineering and High Temperature Chemical Processes--FORTH, University of Patras, Patras, GR-26500, Greece
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1998), (6), 981-990
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
AB Raman spectra of liquid and gaseous ZrCl_4 and of molten ZrCl_4 - CsCl mixts. were measured. Changes of the relative Raman intensities in the vapor phase, near and above the critical point, established the dimerization reaction $2\text{ZrCl}_4(\text{g}) \rightleftharpoons \text{Zr}_2\text{Cl}_8(\text{g})$, $\Delta H^\circ = -56.6 \pm 1.1 \text{ kJ mol}^{-1}$. Spectra of solid and molten Zr chloride show that in the liquid phase ZrCl_4 monomers are present in equilibrium with polymer-like $(\text{ZrCl}_4)_n$ species. A systematic study of the Raman spectra of the solid mixts. formed upon cooling the ZrCl_4 - CsCl melts at different compns. showed that apart from the known Cs_2ZrCl_6 a new compound CsZr_2Cl_9 is also formed. The spectra of solid and molten Cs_2ZrCl_6 and CsZr_2Cl_9 show that ZrCl_6^{2-} and the Zr_2Cl_9^- are present in both phases. In molten ZrCl_4 - CsCl mixts. and at compns. $x\text{ZrCl}_4 < 0.33$ the ZrCl_6^{2-} octahedra are predominant. In the range $0.33 < x\text{ZrCl}_4 < 0.66$ the spectral changes with temperature and composition reflect an equilibrium involving 3 ionic species: ZrCl_6^{2-} , Zr_2Cl_9^- and $\text{Zr}_2\text{Cl}_{10}^{2-}$ (or ZrCl_5^-). At mole fractions rich in ZrCl_4 ($x\text{ZrCl}_4 > 0.66$) the spectra indicate an equilibrium between the ionic Zr_2Cl_9^- , the ZrCl_4 monomer and the $(\text{ZrCl}_4)_n$ polymer-like species. All data suggest that the value of n is small and most probably hexamers and/or dimers are the predominant polymer species in these melts.

RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:74066 CAPLUS
DN 128:115033
TI Hydrocarbon Activation with Metal Halides: Zirconium Tetrachloride Catalyzing the Jacobsen Reaction and Assisting the Trimerization of Alkynes via the Formation of η^6 -Arene-Zirconium(IV) Complexes. [Erratum to document cited in CA127:278262]
AU Musso, Fabrizio; Solari, Euro; Floriani, Carlo; Schenk, Kurt; Chiesi-Villa, Angiola; Rizzoli, Corrado
CS Institut de Chimie Minerale et Analytique BCH, Universite de Lausanne, Lausanne, CH-1015, Switz.
SO Organometallics (1998), 17(2), 274
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
AB The authors Angiola Chiesi-Villa and Corrado Rizzoli were omitted. Kurt

Schenk is affiliated with the Universite de Lausanne; Angiola Chiesi-Villa and Corrado Rizzoli are affiliated with the Universita di Parma.

L4 ANSWER 15 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1997:648897 CAPLUS
DN 127:278262
TI Hydrocarbon Activation with Metal Halides: Zirconium Tetrachloride
Catalyzing the Jacobsen Reaction and Assisting the Trimerization of
Alkynes via the Formation of η^6 -Arene-Zirconium(IV) Complexes
AU Musso, Fabrizio; Solari, Euro; Floriani, Carlo; Schenk, Kurt
CS Institut de Chimie Minerale et Analytique BCH, Universite de Lausanne,
Lausanne, CH-1015, Switz.
SO Organometallics (1997), 16(22), 4889-4895
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
AB Solubilization of the highly insol. polymeric $ZrCl_4$ is achieved using
1,2,4,5-Me₄C₆H₂ (durene) as a carrier in a halogenated solvent, such as
CH₂Cl₂, CHCl₃, 1,2-Dichloroethane, or o-Dichlorobenzene. Solubilization can reach the
level of 40 g of $ZrCl_4$ in 100 mL of CH₂Cl₂ using an equimolar amount of
durene. This is a very successful approach to making available soluble $ZrCl_4$
in a noncoordinating solvent. The solubilization occurs via the formation
of a η^6 -arene complex, which has been structurally characterized in
the form of the hexamethylbenzene derivative [$(\eta^6\text{-Me}_6\text{C}_6)\text{Zr}_2(\mu\text{-Cl})_3\text{Cl}_5$]
(3). This complex is in equilibrium, as revealed by the ¹H NMR spectrum in
CH₂Cl₂, with free C₆Me₆ and a complex (4) which contains a higher Zr/C₆Me₆
ratio. A careful anal. of the CH₂Cl₂ solution, containing originally $ZrCl_4$ and
durene, showed that durene underwent transformation to C₆Me₅H and C₆Me₆.
These species have been trapped, bonded to zirconium in complex
[$(\eta^6\text{-C}_6\text{Me}_5\text{R})\text{Zr}_2(\mu\text{-Cl})_3\text{Cl}_5$] (2, R = H, 50%; R = Me, 50%), which has
been structurally characterized. The Me redistribution reaction in CH₂Cl₂
can result in the inconvenient formation of byproducts derived from the
Zr-assisted Friedel-Craft reaction of CH₂Cl₂ on the arene. The
intermediate of such a reaction has been isolated as [C₆Me₆CHCl₂]+[Zr₂Cl₉]-
(5), whose x-ray structure is available. In order to avoid the
intervention of the solvent and to speed up the reaction, the $ZrCl_4$
rearrangement of methylbenzenes was carried out in neat hydrocarbon at
90° for 6 h. This rearrangement has a number of peculiarities: (i)
unlike the original Jacobsen reaction, it involves intermol. Me transfer;
(ii) it reaches an equilibrium of Me distribution; and (iii) it is catalytic in
zirconium. The very high stability of 3 accounts for the isolation of the
same compound derived from the $ZrCl_4$ -assisted trimerization of 2-butyne in
n-hexane.

RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:679017 CAPLUS
DN 126:25920
TI Synthesis, Structure, and Reactivity of [Zr₆Cl₁₈H₅]²⁻, the First
Paramagnetic Species of Its Class
AU Chen, Linfeng; Cotton, F. Albert
CS Department of Chemistry, Texas A + M University, College Station, TX,
77843, USA
SO Inorganic Chemistry (1996), 35(25), 7364-7369
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
AB Reaction of [Zr₆Cl₁₈H₅]³⁻ (1) with 1 equiv of TiCl₄ yields a new cluster
anion, [Zr₆Cl₁₈H₅]²⁻ (2), which can be converted back into [Zr₆Cl₁₈H₅]³⁻
(1) upon addition of 1 equiv of Na/Hg. Cluster 2 is paramagnetic and
unstable in the presence of donor mols. It undergoes a disproportionation

reaction to form 1, some Zr(IV) compds., and H₂. It also reacts with TiCl₄ to form [Zr₂Cl₉]- (4) and a tetranuclear mixed-metal species, [Zr₂Ti₂Cl₁₆]²⁻ (3). The oxidation reaction of 1 with TiCl₄ is unique. Oxidation of 1 with H⁺ in CH₂Cl₂ solution gave [ZrCl₆]²⁻ (5) and H₂, while in pyridine solution the oxidation product is [ZrCl₅(py)]- (6). There is no reaction between 1 and TiI₄, ZrCl₄, [TiCl₆]²⁻, [ZrCl₆]²⁻, or CrCl₃. [Ph₄P]₂[Zr₆Cl₁₈H₅] (2a), [Ph₄P]₂[Zr₂Ti₂Cl₁₆] (3a), [Ph₄P][Zr₂Cl₉] (4a), [Ph₄P]₂[ZrCl₆]·4MeCN (5a·4MeCN), and [Ph₄P][ZrCl₅(py)] (6a) were characterized by x-ray crystallog. 2A crystallized in the trigonal space group R $\bar{h}3m$ with cell dimensions (20°) of a 28.546(3), b 28.546(3), c 27.679(2) Å, and Z = 12. 3A crystallized in the triclinic space group P $\bar{1}$ with cell dimensions (-60°) of a 11.375(3), b 13.357(3), c 11.336(3) Å, α 106.07(1), β 114.77(1), γ 88.50(1)°, and Z = 1. 4A crystallized in the triclinic space group P $\bar{1}$ with cell dimensions (-60°) of a 12.380(5), b 12.883(5), c 11.000(4) Å, α 110.39(7), β 98.29(7), γ 73.12(4)°, and Z = 2. 5A·4MeCN crystallized in the monoclinic space group P2₁/c with cell dimensions (-60°) of a 9.595(1), b 19.566(3), c 15.049(1) Å, β 98.50(1)°, and Z = 2. 6A crystallized in the monoclinic space group P2₁/c with cell dimensions (20°) of a 10.3390(7), b 16.491(2), c 17.654(2) Å, β 91.542(6)°, and Z = 4.

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:401208 CAPLUS

DN 125:231648

TI Isolated ions ZrF_n⁻ and model dimers [Zr₂F_n]^{m-}

AU Ignat'eva, L. N.; Overchuk, E. I.; Sergienko, V. I.

CS Institut Khimii, Vladivostok, Russia

SO Zhurnal Neorganicheskoi Khimii (1996), 41(3), 496-499

CODEN: ZNOKAQ; ISSN: 0044-457X

PB MAIK Nauka

DT Journal

LA Russian

AB The stability of the fluorozirconate systems ZrF₅⁻, ZrF₆²⁻, ZrF₇³⁻, [Zr₂F₁₁]³⁻, [Zr₂F₁₂]⁴⁻, and [Zr₂F₁₃]⁵⁻ to dissociation through different channels was studied by the X α discrete variation method. The calcns. predict that the ions ZrF₅⁻, ZrF₆²⁻, and [Zr₂F₁₃]⁵⁻ are stable to dissociation. A large pos. charge at the central atom in ZrF₅⁻ makes this ion unstable to the attachment of an addnl. F atom. Highly stable fluorozirconate systems, e.g., [Zr₂F₁₃]⁵⁻, can be formed as polynuclear systems.

L4 ANSWER 18 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:360125 CAPLUS

DN 125:142911

TI η^6 -Arene derivatives of titanium(IV), zirconium(IV) and hafnium(IV)

AU Calderazzo, Fausto; Ferri, Isabella; Pampaloni, Guido; Troyanov, Sergei

CS Universita di Pisa, Dipartimento di Chimica e Chimica Industriale, Sezione di Chimica Inorganica, Via Risorgimento 35, Pisa, I-56126, Italy

SO Journal of Organometallic Chemistry (1996), 518(1-2), 189-196

CODEN: JORCAI; ISSN: 0022-328X

PB Elsevier

DT Journal

LA English

AB The structure of the ionic product [Ti(η^6 -Me₆C₆)Cl₃]₂AlCl₄ 1 has been determined by an x-ray diffraction experiment: orthorhombic; a = 12.890(4), b = 8.609(2), c = 9.168(3) Å; V = 1017.4(6) Å³, Z = 2; d_{calc} = 1.584 g cm⁻³. Tetrachlorogallates of titanium(IV) of general formula [Ti(η^6 -arene)Cl₃]₂GaCl₄ (arene = 1,2,4,5-Me₄C₆H₂, Me₆C₆), have been obtained by reaction of TiCl₄ with the appropriate arene in the presence of GaCl₃ in toluene. Formation of complexes with less methyl-substituted

arene ligands (MeC₆H₅, 1,4-Me₂C₆H₄ and 1,3,5-Me₃C₆H₃) has been established by ¹³C-NMR spectroscopy. The MCl₄/Me₆C₆/benzene system gives, either in the presence or in the absence of aluminum trichloride, covalent (M = Zr) or ionic (M = Hf) compds. of formula Zr(η⁶-Me₆C₆)Cl₂(μ-Cl)₃ZrCl₃ 4 and [Hf(η⁶-Me₆C₆)Cl₃]Hf₂Cl₉ 5. Compds. 4 and 5 have been fully characterized by conventional methods including x-ray crystallog. Compound 5: orthorhombic; a = 17.662(6), b = 8.960(3), c = 17.683(6) Å; V = 2798.4(16) Å³, Z = 4; d_{calc} = 2.666 g cm⁻³.

L4 ANSWER 19 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:198411 CAPLUS

DN 114:198411

TI Synthesis, thermal decomposition and vibrational spectra of hydrazinium(1+) heptafluorozirconate(IV) and hafnate(IV)

AU Rahten, A.; Milicev, S.

CS "J. Stefan" Inst., Ljubljana, Yugoslavia

SO Thermochimica Acta (1990), 171, 185-92

CODEN: THACAS; ISSN: 0040-6031

DT Journal

LA English

AB (N₂H₅)₃MF₇ (M = Zr, Hf) were synthesized from aqueous solns. of (N₂H₆)₃M₂F₁₃.F and N₂H₄.H₂O. IR and Raman spectra show the presence of a dimeric or polymeric anion with a coordination number >6, and 2 types of N₂H₅⁺, involved predominantly through their NH₃⁺ groups in weak H bonds. On heating, the compds. start to lose weight >120° (Zr compound) or >110° (Hf compound). Decomposition proceeds through (NH₄)₂MF₆ and NH₄MF₅ (γ-NH₄ZrF₅) to MF₄ (predominantly α-ZrF₄), and finishes at .apprx.350° (Zr compound) or .apprx.380° (Hf compound). Raman spectra of decomposition intermediates show that the composite anionic part transforms through other complex or polymeric fluorozirconate(IV) or hafnate(IV) anions to MF₄, and no simple MF₆²⁻ or MF₅⁻ appear.

L4 ANSWER 20 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:198403 CAPLUS

DN 114:198403

TI Tellurium cations by Lewis acid-base reactions: syntheses and crystal structures of (Te₄²⁺)(Zr₂Br₁₀²⁻) and (TeBr₃⁺)(Zr₂Br₉⁻)

AU Beck, Johannes

CS Inst. Anorg. Chem., Univ. Karlsruhe, Karlsruhe, D-7500/1, Germany

SO Chemische Berichte (1991), 124(4), 677-81

CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA English

AB ZrBr₄ reacts with Te₂Br at 210° in quant. yield to afford (Te₄²⁺)(Zr₂Br₁₀²⁻) as blue-black, moisture-sensitive crystals. The crystal structure determination shows that (Te₄)(Zr₂Br₁₀) consists of planar, nearly square Te₄²⁺ and Zr₂Br₁₀²⁻ ions, that form edge-sharing double octahedra. Both ions possess crystallog. 2/m (C_{2h}) symmetry. At > 250° (Te₄)(Zr₂Br₁₀) decomp. with cleavage of Te-Te bonds into (TeBr₃⁺)(Zr₂Br₉⁻), which forms yellow, hygroscopic crystals. (TeBr₃)(Zr₂Br₉) can also be obtained by the reaction of 2 equiv of ZrBr₄ with TeBr₄ at 260°. Its crystal structure is built of Zr₂Br₉⁻ ions, that form face-sharing double octahedra, and of pyramidal TeBr₃⁺ ions, resulting in a strongly deformed octahedral coordination for the Te atom. The Zr₂Br₉ double octahedra and the TeCl₆ octahedra are connected by common edges and corners to infinite chains. (Te₄)(Zr₂Br₁₀) and (TeBr₃)(Zr₂Br₉) are monoclinic, space groups I₂/m and P₂1/c, Z = 4, R/R_w = 0.041/0.031 and 0.045/0.036, resp.

L4 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1990:451378 CAPLUS

DN 113:51378

TI Fluoro- and oxofluorozirconates

AU Sengupta, A. K.; Bhattacharyya, U.

CS Dep. Chem., Kalyani Univ., Kalyani, 741 235, India
 SO Journal of Fluorine Chemistry (1990), 46(2), 229-41
 CODEN: JFLCAR; ISSN: 0022-1139
 DT Journal
 LA English
 AB The preps. of (LH₂)[ZrF₃].mH₂O (L = ethylenediamine (m = 0) and biguanide (m = 1)), (L₁H)₂[ZrF₆].nH₂O (L₁ = guanidine (n = 1), pyridine (py) (n = 0)), (L₂H)[ZrF₆].H₂O (L₂ = α-, β-, and γ-picoline (pic)), (L₃H₂)[ZrOF₃].2.xH₂O (L₃ = ethylenediamine (x = 5), propylene-1,2-diamine (x = 3), N,N'-dimethylethylenediamine (x = 3)), MI[ZrOF₃].1.5H₂O (MI = alkali metals), (N₂H₅)[Zr₂O₂F₅].4H₂O and (L₄H₂)[ZrOF₄] (L₄ = 1,10-phenanthroline and 2,2'-bipyridine) are described. The compds. were characterized by chemical anal., TGA, IR spectroscopy and x-ray powder photog. The (pyH)₂[ZrF₆] is unstable and undergoes slow decomposition on keeping in air. On isothermal heating at 120° it yields (pyH)[ZrF₅]. At 180° (α-picH)[ZrF₅].H₂O yields (α-picH)[Zr₂F₉]. K[ZrOF₃].1.5H₂O yields K[ZrOF₃].0.5H₂O and the anhydrous compound successively at 130 and 225°, resp. The corresponding anhydrous Cs compound is produced at 220°. IR spectra suggest the presence of Zr-O-Zr chains in the oxofluoro compds. From the various types of studies it appears that the oxofluorozirconates contain only a fraction of water as Zr-OH group.

L4 ANSWER 22 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1990:227069 CAPLUS
 DN 112:227069
 TI Crystal structure and vibrational spectra of hydrazinium(2+) tri-μ-fluorobis[pentafluorozirconate(IV)] fluoride and vibrational spectra of its hafnium analog
 AU Rahten, A.; Leban, I.; Milicev, S.; Zemva, B.
 CS "J. Stefan" Inst., E. Kardelj Univ., Ljubljana, Yugoslavia
 SO Journal of Crystallographic and Spectroscopic Research (1990), 20(1), 9-15
 CODEN: JCREDB; ISSN: 0277-8068
 DT Journal
 LA English
 AB The title Zr compound is monoclinic, space group P2₁, with a 5.670(1), b 10.984(2), c 10.601(2) Å, and β 93.88(1)°; dc = 2.776 for Z = 2. The final R = 0.0205 and Rw = 0.0294 for 2003 reflections. Atomic coordinates are given. Two different types of N₂H₆²⁺ ions are present. One is involved in strong H-bonds to F⁻ in infinite chains running along the a-axis, and the other links the structure through weaker bi- and trifurcated H-bonds to F ligands of the Zr₂F₁₃⁻ ions. The Zr₂F₁₃⁻ ions have very nearly C₂ point symmetry and are formed by joining 2 distorted bicapped trigonal prisms of ZrF₈-units through a common face. The vibrational spectra of the Zr and its Hf analog are nearly identical, with the exception of a strong IR band, which is assigned to a stretching mode of the moving central atom within the anion. The anion part of the spectrum is simple, showing broad unresolved bands. The cation part shows 2 types of N₂H₆²⁺ ions. H-bonding is strongly present in the spectra, but no simple correlations with the H-bond strength is evident.

L4 ANSWER 23 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1984:521874 CAPLUS
 DN 101:121874
 TI Metal chloride-phosphorus chloride-alkyl chloride complexes: reactions with gold(III), zirconium(IV), platinum(IV) and oxouranium(VI) chlorides
 AU Lata, Sneha; Dubey, S. N.; Puri, D. M.
 CS Chem. Dep., Kurukshetra Univ., Kurukshetra, 132 119, India
 SO Journal of the Indian Chemical Society (1983), 60(10), 911-13
 CODEN: JICSAH; ISSN: 0019-4522
 DT Journal
 LA English
 AB [R₃PCl₃]_x (R = tert-Bu, tert-amyl, cyclohexyl, triphenylmethyl; X = AuCl₄, Zr₂Cl₉, 0.5 PtCl₆, 0.5 UO₂Cl₄) and [R₃PCl₂Ph]_z (Z = AuCl₄, Zr₂Cl₉, 0.5

UO₂Cl₄) were prepared from HAuCl₄, ZrCl₄, H₂PtCl₆, or UO₂Cl₂ and PCl₃ or PCl₂Ph and RCl. The products were characterized by elemental anal., thermogravimetric anal., elec. conductivity, magnetic susceptibility, and IR

and

electronic spectral methods.

L4 ANSWER 24 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1983:529309 CAPLUS
DN 99:129309
TI TDPAC investigation on ammonium hafnium fluoride (NH₄Hf₂F₉)
AU Martinez, J. A.; Caracoche, M. C.; Rodriguez, A. M.; Rivas, P. C.; Lopez Garcia, A. R.
CS Fac. Cienc. Exactas, Univ. Nac. La Plata, La Plata, 1900, Argent.
SO Hyperfine Interactions (1983), 14(2), 135-8
CODEN: HYINDN; ISSN: 0304-3843
DT Journal
LA English
AB Time-differential perturbed angular correlation (TDPAC) measurements in NH₄Hf₂F₉ [87118-39-6] were performed between 15 and 580 K. The compound was stable in the whole temperature range and no phase transitions were observed. Exptl. results could be explained by assuming 2 equally populated quadrupole interactions which suggest an inequivalence between the 2 sites occupied by the Hf atoms in the mol.

L4 ANSWER 25 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1983:79040 CAPLUS
DN 98:79040
TI Activities in systems based on alkali metal fluorides and tetrafluorides. I. Metal fluoride-zirconium tetrafluoride systems
AU Sidorov, L. N.; Pozdyshkina, O. V.; Zhuravleva, L. V.; Korenev, Yu. M.
CS Mosk. Gos. Univ., Moscow, USSR
SO Deposited Doc. (1982), VINITI 58-82, 37 pp. Avail.: VINITI
DT Report
LA Russian
AB Activities were calculated in MF-ZrF₄ (M = Li, Na, K, Rb, Cs) melts from heats of melting of the components and M₃ZrF₇ combined with published mass spectral values for partial pressures over these melts. Equilibrium consts. and heats and entropies of formation of MZrF₅, M₂ZrF₆, M₃ZrF₇, and MZr₂F₉ were calculated at 800-1300 K.

L4 ANSWER 26 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1983:79038 CAPLUS
DN 98:79038
TI Activities in systems based on alkali metal fluorides and tetrafluorides. II. Metal fluoride-hafnium tetrafluoride systems
AU Zhuravleva, L. V.; Pozdyshkina, O. V.; Sidorov, L. N.
CS Khim. Fak., Mosk. Gos. Univ., Moscow, USSR
SO Deposited Doc. (1982), VINITI 59-82, 15 pp. Avail.: VINITI
DT Report
LA Russian
AB Extrapolation of activity values for MF-ZrF₄ (M = Li, Na, K, Rb, Cs) systems along with estimated values for heats of melting of HfF₄ enabled calcn. of activities in the MF-HfF₄ systems at 1155 K. Equilibrium consts. and heats and entropies of formation were calculated for MHfF₅, M₂HfF₆, M₃HfF₇, and MHf₂F₉ at 800-1200 K.

L4 ANSWER 27 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1982:589075 CAPLUS
DN 97:189075
TI Mass spectrometric determination of the enthalpies of dissociation of gaseous complex fluorides into neutral and charged particles. VI. Enthalpy of formation of pentafluorozirconate (ZrF₅-)
AU Skokan, E. V.; Sorokin, I. D.; Sidorov, L. N.; Nikitin, M. I.

CS Dep. Chem., Moscow State Univ., Moscow, 117234, USSR
 SO International Journal of Mass Spectrometry and Ion Physics (1982), 43(4), 309-25
 CODEN: IJMIBY; ISSN: 0020-7381
 DT Journal
 LA English
 AB Effusion and mass spectroscopic methods were used to study the ion/mol. equilibrium involving neg ions ZrF_5^- and Zr_2F_9^- . The heats of the reactions: $\text{ZrF}_4 + \text{F}^- \rightarrow \text{ZrF}_5^-$ and $\text{ZrF}_4 + \text{ZrF}_5^- \rightarrow \text{Zr}_2\text{F}_9^-$ were determined at 298.15 K, from which the heats of formation were derived. By using these values and information from the literature, heats of formation and mol. consts. were estimated for MZrF_5 and MZr_2F_9 (M is an alkali metal) and their heats of dissociation into ions were calculated

L4 ANSWER 28 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1982:479745 CAPLUS
 DN 97:79745
 TI Synthesis and characterization of some binary and ternary zirconium iodides
 AU Guthrie, D. H.
 CS Ames Lab., Ames, IA, USA
 SO Report (1981), IS-T-958; Order No. DE82005452, 125 pp. Avail.: NTIS From: Energy Res. Abstr. 1982, 7(8), Abstr. No. 22652
 DT Report
 LA English
 AB Studies of binary $\text{ZrI}_4\text{-Zr}$ and ternary CsI-Zr-ZrI_4 systems produced several new compds. The new binary compds. include two polymorphs of ZrI_2 (α and β) as well as a phase described earlier as $\text{ZrI}_{1.8}$. $\alpha\text{-ZrI}_2$ is monoclinic space group $\text{P}2_1/\text{m}$ with a 6.821(2), b 3.741(1), c 14.937(3) Å, and β 95.66(3)°; $Z = 4$ ($R = 0.064$). $\beta\text{-ZrI}_2$ is trigonal, space group $\text{R}\bar{3}\text{m}$, with hexagonal axes a 14.502(2) and c 9.996(2) Å; $Z = 18$ ($R = 0.109$). This phase contains a Zr_6I_{12} cluster. Guinier x-ray powder diffraction data previously reported for $\text{ZrI}_{1.8}$ has now been found to arise from $\alpha\text{-ZrI}_2$ intergrown with an orthorhombic ZrI_2 phase (perhaps isostructural with WTe_2 plus an unknown phase. The ternary compds. include Cs_2ZrI_6 , $\text{Cs}_3\text{Zr}_2\text{I}_9$, and $\text{Cs}_3\text{Zr}_6\text{I}_{14}$. The first is isostructural with K_2PtCl_6 . $\text{Cs}_3\text{Zr}_2\text{I}_9$ belongs to space group $\text{P}6_3/\text{mmc}$ with a 8.269(1) and c 19.908(3) Å; $Z = 2$. This phase has a $\text{Cs}_3\text{Cr}_2\text{Cl}_9$ -type structure, with Zr-Zr distance of 3.134(4) Å ($R = 0.087$). Crystals of $\text{Cs}_3\text{Zr}_6\text{I}_{14}$ is orthorhombic, space group Cc , with a 14.275(4), b 15.880(4), and c 12.953(4) Å ($R = 0.062$). This phase also contains a Zr_6I_{12} cluster.

L4 ANSWER 29 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1982:110997 CAPLUS
 DN 96:110997
 TI Mass-spectrometric study of (potassium fluoride + zirconium tetrafluoride) and cesium fluoride + zirconium tetrafluoride). Molecular composition of vapor, activities, and congruent and incongruent sublimation of 3KF.ZrF_4 crystal
 AU Sidorov, L. N.; Karasev, N. M.; Korenev, Yu. M.
 CS Dep. Chem., Moscow State Univ., Moscow, 117234, USSR
 SO Journal of Chemical Thermodynamics (1981), 13(10), 915-35
 CODEN: JCTDAF; ISSN: 0021-9614
 DT Journal
 LA English
 AB The Knudsen-effusion method was used together with mass-spectrometric anal. of evaporation products to study $\text{KF} + \text{ZrF}_4$ and $\text{CsF} + \text{ZrF}_4$ systems. The mols. MZrF_5 , MZr_2F_9 , and M_2ZrF_6 (M = alkali metal) were found in the gas phase and their partial pressures and enthalpies of dissociation were obtained. Activities of pure components were determined at 1165 K. The solid compound 3KF.ZrF_4 , which melts congruently at 1197 K, sublimes congruently only ≤ 1103 K.

L4 ANSWER 30 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1981:165889 CAPLUS
 DN 94:165889
 TI Metal-metal repulsion and bonding in confacial bioctahedra. The crystal structures of cesium yttrium iodide (Cs₃Y₂I₉) and cesium zirconium iodide (Cs₃Zr₂I₉) and comparison with related phases
 AU Guthrie, Dennis H.; Meyer, Gerd; Corbett, John D.
 CS Ames Lab., Iowa State Univ., Ames, IA, 50011, USA
 SO Inorganic Chemistry (1981), 20(4), 1192-6
 CODEN: INOCAJ; ISSN: 0020-1669
 DT Journal
 LA English
 AB The title compds. were synthesized by reaction of CsI₃ and Y or CsI, Zr, and ZrI₄ at 750-850° in welded Ta containers. Both have the Cs₃Cr₂Cl₉-type structure, space group P6₃/mmc, with a 8.406(1), 8.269(1) and c 21.280(5), 19.908(3); R = 0.050, 0.082, R_w = 0.082, 0.077 for Cs₃Y₂I₉ and Cs₃Zr₂I₉, resp. The transition from the Y to the Zr compound is accompanied by a decrease of the metal-metal distance in the M₂I₉-confacial bioctahedra from 4.052(9) to 3.129(4) Å due to the formation of a Zr-Zr bond. Correspondingly large changes occur in the internal angles in the M-I-M bridges. Parameters of 5 M₂X₉ groups in the Cs₃Cr₂Cl₉-type structure and CsCdCl₃, all of which lack M-M bonds, are considered in terms of a model which recognizes the existence of both longer M-X bridge bonds and compromise bridge angles. Nonbonding repulsion between M atoms is not a significant factor in these structures. The effects of packing and metal-metal bonding are also considered.

L4 ANSWER 31 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1981:21167 CAPLUS
 DN 94:21167
 TI Application of high temperature mass spectrometry to the investigation of P-T-X phase diagrams
 AU Korenev, Yu. M.
 CS Dep. Chem., Moscow State Univ., Moscow, 117234, USSR
 SO Advances in Mass Spectrometry (1980), 8A, 458-61
 CODEN: AMSPA; ISSN: 0568-000X
 DT Journal
 LA English
 AB High temperature mass spectroscopy was used to study the phase diagrams of the alkali metal-HfF₄ and -ZrF₄ systems. The partial pressures of all the mols. present in the vapor phase over the whole range of concentration as well as their heats of evaporation were determined. In addition, dissociation enthalpies and entropies of the complex mols. formed were determined. The gaseous phase composition and the total pressures at the temperature and concentration corresponding to the lines of the 3-phase equilibrium were calculated to construct the T-X and P-T projections of the phase diagram of the system.

L4 ANSWER 32 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1980:574608 CAPLUS
 DN 93:174608
 TI T-x and P-T projections of a rubidium fluoride-zirconium fluoride system phase diagram
 AU Korenev, Yu. M.; Skokan, E. V.; Karasev, N. M.; Akishin, P. A.
 CS Mosk. Gos. Univ., Moscow, USSR
 SO Vestnik Moskovskogo Universiteta, Seriya 2: Khimiya (1980), 21(4), 400
 CODEN: VMUKA5; ISSN: 0579-9384
 DT Journal
 LA Russian
 AB A Knudsen effusion-mass spectral study at 839-1094 K showed that the vapor

over RbF-ZrF₄ systems containing 33.3-61.5 mol % ZrF₄ contains RbF, ZrF₄, RbZrF₅, Rb₂ZrF₆, and RbZr₂F₉. Partial pressures, heats of evaporation, and heats of dissociation were determined (RbZrF₅ = RbF + ZrF₄, $\Delta H^\circ_{1094K} = 62.6 \pm 2.6$; Rb₂ZrF₆ = RbF + RbezrF₅, 45.4 ± 3.6 ; RbZr₂F₉ = RbZrF₅ + ZrF₄, $\Delta H^\circ_{839K} = 42.4 \pm 6$ kcal/mol). Temperature-composition and pressure-temperature diagrams were constructed.

L4 ANSWER 33 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1980:432482 CAPLUS
DN 93:32482
TI P-T and T-x projections of a phase diagram of the cesium fluoride-zirconium fluoride system
AU Karasev, N. M.; Korenev, Yu. M.; Sidorov, L. N.
CS USSR
SO Zhurnal Neorganicheskoi Khimii (1980), 25(5), 1362-7
CODEN: ZNOKAQ; ISSN: 0044-457X
DT Journal
LA Russian
AB A Knudsen effusion-mass spectral study of evaporation products in the CsF-ZrF₄ system showed formation of CsF, Cs₂F₂, ZrF₄, Cs₂ZrF₆, CsZrF₅, and CsZr₂F₉. Heats of evaporation and partial pressures of vapor species were determined as a function of melt composition. Heats of dissociation of CsZrF₅, Cs₂ZrF₆, and CsZr₂F₉ are 59.6 ± 2.6 , 42.6 ± 4.0 , and 44.3 ± 4.0 kcal/mol, resp. The pressure-temperature and temperature-composition phase diagrams are given.

L4 ANSWER 34 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1980:153753 CAPLUS
DN 92:153753
TI Molecular composition of vapor in a sodium fluoride-zirconium fluoride system
AU Korenev, Yu. M.; Sidorov, L. N.; Rykov, A. N.; Novoselova, A. V.
CS USSR
SO Zhurnal Neorganicheskoi Khimii (1980), 25(1), 284-90
CODEN: ZNOKAQ; ISSN: 0044-457X
DT Journal
LA Russian
AB A combination Knudsen effusion-mass spectral study showed formation of Na₂ZrF₆, NaZrF₅, (NaZrF₅)₂, and NaZr₂F₉ in the vapor phase. Partial pressures of all vapor components were determined and then used (along with heats of evaporation) to calculate vapor compns. and to construct T-x and P-T diagrams for the NaF-ZrF₄ system.

L4 ANSWER 35 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1980:47966 CAPLUS
DN 92:47966
TI Use of a mass spectral method to construct P-T and T-x projections of the phase diagram of lithium fluoride-zirconium tetrafluoride system
AU Korenev, Yu. M.; Rykov, A. N.; Novoselova, A. V.
CS Mosk. Gos. Univ., Moscow, USSR
SO Zhurnal Neorganicheskoi Khimii (1979), 24(8), 2201-7
CODEN: ZNOKAQ; ISSN: 0044-457X
DT Journal
LA Russian
AB Compns. and vapor pressures were determined by Knudsen effusion-mass spectral anal. methods. The saturated vapor contains LiF, Li₂F₂, Li₃F₃, ZrF₄, LiZrF₅, Li₂ZrF₆, and LiZr₂F₉. Heats of vaporization and partial pressures were calculated as a function of melt composition. Heats of dissociation of LiZrF₅, Li₂ZrF₆, and LiZr₂F₉ are 55.0 ± 3.0 , 56.2 ± 3.5 , and 40.3 ± 3.0 kcal/mol, resp.

L4 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1979:77198 CAPLUS
 DN 90:77198
 TI Pressure-temperature and temperature-composition projections of the phase diagram of a cesium fluoride-hafnium tetrafluoride system
 AU Loshin, A. F.; Korenev, Yu. M.; Novoselova, A. V.
 CS USSR
 SO Deposited Doc. (1977), VINITI 2462-77, 27 pp. Avail.: VINITI
 DT Report
 LA Russian
 AB Vapor composition of the CsF-HfF₄ system was studied by mass spectroscopy. Formation of CsHfF₅ and CsHf₂F₉ is indicated, but not Cs₂HfF₆ (in vapor phase). Entropies of dissociation of CsHfF₅ and CsHf₂F₉ are 32 and 30 entropy units, resp., and heats of dissociation are 59.7 ± 3.0 and 44.4 ± 4.0 , resp. Heats of vaporization of HfF₄, CsHfF₅, and CsHf₂F₉ were calculated for various melt compns. Activities and free energies of formation of melts of CsF and HfF₄ at various compns. are given.

L4 ANSWER 37 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1976:549834 CAPLUS
 DN 85:149834
 TI Partial pressures, activities, and heats of evaporation in the potassium fluoride-zirconium fluoride system
 AU Karasev, N. M.; Sidorov, L. N.; Korenev, Yu. M.
 CS Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR
 SO Zhurnal Fizicheskoi Khimii (1976), 50(6), 1629
 CODEN: ZFKHA9; ISSN: 0044-4537
 DT Journal
 LA Russian
 AB The composition of the vapors over the complex mols. KZrF₅, K₂ZrF₆ and KZr₂F₉ were determined by the Knudsen effusion method in combination with mass spectrometry. The partial pressures of these complex mols. and the partial pressure and activities of KF [7789-23-3] and ZrF₄ [7783-64-4] in the vapor phase were determined. The heats of dissociation at 1165°K of these complex mols. were calculated from the activities, heats of evaporation and equilibrium consts. for the dissociation reactions.

L4 ANSWER 38 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1976:499966 CAPLUS
 DN 85:99966
 TI Molecular composition of vapor and interpretation of mass spectrum in potassium fluoride-zirconium fluoride and cesium fluoride-zirconium fluoride systems
 AU Karasev, N. M.; Sidorov, L. N.; Korenev, Yu. M.
 CS Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR
 SO Zhurnal Fizicheskoi Khimii (1976), 50(6), 1630
 CODEN: ZFKHA9; ISSN: 0044-4537
 DT Journal
 LA Russian
 AB A Knudsen effusion method using mass spectral anal. was used to determine the vapor composition over ZrF₄-MF (M = K, Cs) melts. The vapor contains MZrF₅, MZr₂F₉, and traces of M₂ZrF₆ as well as the initial components.

L4 ANSWER 39 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1974:544914 CAPLUS
 DN 81:144914
 TI Metal halide-phosphorus halide-alkyl halide complexes. III. μ -Trihalohexahalodimetallate ions of titanium and zirconium
 AU Bullock, Joseph I.; Parrett, Frederick W.; Taylor, Nicholas J.
 CS Dep. Chem., Univ. Surrey, Surrey, UK
 SO Canadian Journal of Chemistry (1974), 52(16), 2880-8
 CODEN: CJCHAG; ISSN: 0008-4042
 DT Journal

LA English

AB TiCl_4 reacted rapidly with PCl_3 , PBr_3 , and MePCl_2 in the presence of Me_3CCl to give compds. containing a phosphonium cation, $\text{R}_1\text{R}_2\text{PX}_2^+$ ($\text{R}_1 = \text{Me}_3\text{C}$; $\text{R}_2 = \text{Cl}$, Br , or Me ; $\text{X} = \text{Cl}$ or Br), and the principal metal-containing anion, Ti_2Cl_9^- . For PBr_3 and Me_3CCl , a stoichiometric product, $[\text{Me}_3\text{CPBr}_3][\text{Ti}_2\text{Cl}_9]$ was obtained which was characterized by using vibrational spectroscopy. The other reactions gave nonstoichiometric materials, the sublimates of which may contain higher polymeric anions; the residues contained TiCl_5^- along with the parent dimeric anion. ZrCl_4 and TiBr_4 reacted in a similar way to give Zr_2Cl_9^- and Ti_2Br_9^- in stoichiometric reactions.

L4 ANSWER 40 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1959:37873 CAPLUS

DN 53:37873

OREF 53:6742g-i

TI Vapor pressures and molecular composition of vapors of the RbF-ZrF_4 and LiF-ZrF_4 systems

AU Sense, Karl A.; Stone, Richard W.

CS Battelle Mem. Inst., Columbus, O.

SO Journal of Physical Chemistry (1958), 62, 1411-18
CODEN: JPCHAX; ISSN: 0022-3654

DT Journal

LA Unavailable

AB The vapor pressure of RbF at $798\text{--}1059^\circ$ is given by $\log p(\text{mm.}) = 63 - 17,722/T - 15.66 \log T$ and at $589\text{--}798^\circ$ by $\log p(\text{mm.}) = 10.263 - 11,266/T$. The vapor pressure of LiF at $850\text{--}1060^\circ$ is given by $\log p(\text{mm.}) = 8.797 - 11,409/T$. Vapor pressures of the RbF-ZrF_4 and LiF-ZrF_4 systems were measured over the ranges $690\text{--}1060$ and $670\text{--}1060^\circ$, resp. The complexes RbZr_2F_9 and LiZr_2F_9 exist in the vapor phases. Further work on the NaF-ZrF_4 system points to the existence of the gaseous complex NaZr_2F_9 rather than NaZrF_5 as previously supposed (C.A. 52, 14308h). A phase diagram of the RbF-ZrF_4 system derived from vapor-pressure data showed a constant b.p. to exist at about 33 mole % ZrF_4 for a total pressure of 1 mm. Plots showing the change of total pressure with composition for various temps., as well as m.p. curves, were given for the various systems.

L4 ANSWER 41 OF 41 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1957:88941 CAPLUS

DN 51:88941

OREF 51:16068e-h

TI Vapor pressures of the rubidium fluoride-zirconium fluoride and lithium fluoride-zirconium fluoride systems

AU Sense, Karl A.; Stone, Richard W.; Filbert, Robert B., Jr.

CS Battelle Mem. Inst., Columbus, O.

SO U.S. Atomic Energy Comm. (1957), BMI-1199, 35 pp.

DT Journal

LA Unavailable

AB The vapor pressures of RbF and LiF were determined in the temperature range of 589 to

1059° and 851 to 1060° , resp. The pressure-temperature relations for solid RbF were expressed by an equation: $\log p = 10.263 - (11,226/T)$. Liquid RbF results were best expressed by the equation: $\log p = 63.823 - (17,772/T) - 15.660 \log T$. The m.p. of RbF could not be determined with any degree of certainty from these data alone; however, the m.p. of RbF was found to be 798° by thermal analysis. The vapor-pressure data obtained for LiF in the temperature range of 851 to 1060° was expressed by the equation: $\log p = 8.797 - (11,409/T)$. Vapor pressures of the RbF-ZrF_4 and LiF-ZrF_4 systems were measured over the temperature ranges of 690 to 1060° and 670 to 1060° , resp. The complexes RbZr_2F_9 and LiZr_2F_9 were believed to exist in the vapor phase of the respective systems. A more detailed examination of the NaF-ZrF_4 system indicated that the vapor-phase complex NaZr_2F_9 exists, rather than NaZrF_5 , as previously

supposed. Vapor-pressure data were used to construct a phase diagram for the RbF-ZrF₄ system at a total pressure of 1 mm. of Hg. A constant b.p. was found at approx. 33 1/3 mole % ZrF₄.

(FILE 'HOME' ENTERED AT 13:50:38 ON 21 AUG 2006)

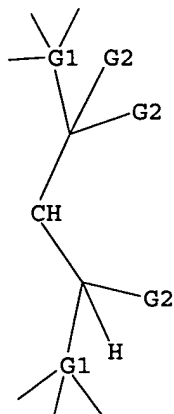
FILE 'REGISTRY' ENTERED AT 13:51:02 ON 21 AUG 2006

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 Si,Ge,Pb,Sn

G2 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Ph,H

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 13:51:26 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 12052 TO ITERATE

16.6% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

6 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 234463 TO 247617
PROJECTED ANSWERS: 363 TO 1083

L2 6 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 13:51:32 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 239601 TO ITERATE

100.0% PROCESSED 239601 ITERATIONS (1 INCOMPLETE)
SEARCH TIME: 00.00.02

528 ANSWERS

L3 528 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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167.15

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=> s l3

L4 373 L3

=> s l4 and py<2002

21829994 PY<2002

L5 275 L4 AND PY<2002

=> s l5 and cation#

378631 CATION#

L6 3 L5 AND CATION#

=> d 1-3 bib abs

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1979:86393 CAPLUS

DN 90:86393

TI Radical ions. XXVIII. Tris(trimethylsilylmethyl)aminium,
.ovrhdot.+N(CH₂Si(CH₃)₃)₃: a stable fluxional aminium radical
cation

AU Bock, Hans; Kaim, Wolfgang; Kira, Mitsuo; Osawa, H.; Sakurai, H.

CS Inst. Inorg. Chem., Univ. Frankfurt, Frankfurt/Main, Fed. Rep. Ger.

SO Journal of Organometallic Chemistry (1978), 164(3), 295-304

CODEN: JORCAI; ISSN: 0022-328X

DT Journal

LA English

AB The 1st ionization potentials of 11 R₃-nN(CH₂SiMe₂)_n, determined by photoelectron spectroscopy, are 7.66-9.07 eV. The most easily ionized mol., N(CH₂SiMe₃)₃, can also be oxidized with AlCl₃ in CH₂Cl₂ to its aminium radical cation. The ESR spectra at 180-310 K display a strong temperature dependence due to rotations about the N-CH₂ bonds.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1972:33675 CAPLUS

DN 76:33675

TI σ - π Conjugation of carbon-metal bonds. Dehydrometalation of
alkylmetal compounds

AU Jerkunica, Josko M.; Traylor, T. G.

CS Revelle Coll., Univ. California, La Jolla, CA, USA

SO Journal of the American Chemical Society (1971), 93(23), 6278-9

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English
 AB Ph₃CBF₄ was treated with Me₂EtSn in CH₂Cl₂. The trityl cation spectrum disappeared almost immediately and Ph₃CH, CH:CH₂, and Me₃SnBF₄ were produced in nearly quant. yields. Similar reactions occurred with Bu₂Hg, PhCH₂CH₂PbPh₃, (PhCH₂CMeH)₂Hg and PhCMeHSnMe₃. However, PhCH₂SnMe₃, Me₄Sn, (PhCMe₂CH₂)₂Hg and bis(1-apocamphyl)mercury did not react, illustrating the importance of the presence and proper geometry of the βH. A large variation in rate with the nature of the metal was in keeping with predictions based on σ- π conjugation effects.

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1959:88875 CAPLUS
 DN 53:88875
 OREF 53:15955b-f
 TI Unsymmetrical dialkylphosphinic acids
 AU Crofts, P. C.; Fox, I. S.
 CS Manchester Coll. Sci. Technol.
 SO Journal of the Chemical Society (1958) 2995-7
 CODEN: JCSOA9; ISSN: 0368-1769
 DT Journal
 LA Unavailable
 OS CASREACT 53:88875
 AB Four unsym. RR'PO₂H, where R and R' are combinations of Me, Et, iso-Pr, and tert-Bu groups, were made by reaction of RMgX with a blocked or sterically hindered R'POCl₂. EtPOCl₂ (I) was made by NaI isomerization of (EtO)₃P, hydrolysis using refluxing aqueous HCl, and treatment of the EtPO₃H₂ with SOCl₂ at reflux for 3 h. Adding 90 mL. of a solution of 0.2 mol Me₂NH in 30-40° petr. ether over 20 min. to a stirred solution of 14.7 g. I in 200 mL. 30-40° petr. ether, filtering off Me₂NH.HCl, and distilling the filtrate gave 10.5 g Et(Me₂N)POCl (II), b₁₀ 102°. Adding 24.2 g. II in 100 mL. Et₂ to MeMgBr (from 4.8 g. Mg) in 70 mL. Et₂O over 2 h., refluxing 4 h., acidifying with 100 mL. concentrated HCl and 100 mL. H₂O, distilling the ether, evaporating the aqueous solution, refluxing the residue in 100 mL. concentrated HCl overnight, evaporating, drying in vacuo over KOH pellets, passing an aqueous solution through a cation-exchange column, and concentrating effluent in vacuo gave a yellow oil which on distilling gave 14.6 g. crude EtMePO₂H; careful refractionation gave 2.5 g., b₁₁ 170-2°, m. 7-8°, n_{20D} 1.4514. Similarly 21.8 g. II with iso-PrMgCl (III) gave 6.0 g. Et(iso-Pr)PO₂H, b_{0.017} 89.5°, n_{20D} 1.4567. Iso-PrPOCl₂ (16.0 g.) gave 13.2 g. iso-Pr-(Me₂N)POCl, b₁₂ 104°, n_{25D} 1.4628, 17.0 g. of which with Me₂MgCl similarly gave 7.0 g. Me(iso-Pr)PO₂H, b_{0.05} 96-8°, n_{24D} 1.4502. tert-BuPOCl₂ (IV) was sufficiently hindered to react selectively with III. Adding 17.0 g. IV in 100 mL. Et₂O over 30 min. to III (from 10.0 g. iso-PrCl) in 150 mL. Et₂O gave 2.7 g. crude acid, which on 5 recrystns. gave 0.8 g. tert-Bu(iso-Pr)PO₂H, m. 82-4° (petr. ether).

=> s 15 and salts
 597843 SALTS
 L7 2 L5 AND SALTS

=> d 1-2 bib abs

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1998:352139 CAPLUS
 DN 129:95608
 TI Preparation of 2-amino-1,3-propanediols and their use as immunosuppressants
 IN Shimazaki, Norihiko; Kayagiri, Hiroshi; Fukami, Naoki; Watanabe, Shinya; Yoshimura, Seiji; Abe, Yoshito; Mizutani, Takeshi

PA Fujisawa Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 63 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT.1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10147587	A2	19980602	JP 1997-315534	19971117 <--
PRAI	AU 1996-3716	A	19961119		
	AU 1997-6948	A	19970523		
OS	MARPAT 129:95608				
AB	R2R3R4SiAEGJLC(NHR1)(CH2OH)2 [R1 = H, acyl; R2 = H, lower alkyl, aryl; R3 = H, alkyl; R2R3 may form linear or branched lower alkylene; R4 = H, (halo)alkyl, alkenyl, (un)substituted aryl, heterocyclyl, etc.; A = alkylene; E = bond, O, imino; G = bond, arylene; J = bond, O; L = bond, lower alkene] and their medically acceptable salts are prepared The compds. are useful for treatment of autoimmune disease, psoriasis, rejection, etc. Hydrolysis of 2-acetamido-2-[2-[4-[4-(dimethylphenylsilyl)butoxy]phenyl]ethyl]-1,3-propanediol and subsequent HCl salt formation gave HCl salt of the corresponding amine derivative, which showed strong immunosuppressive activity.				

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1958:10901 CAPLUS
DN 52:10901

OREF 52:1917f-i,1918a

TI The addition of trichlorosilane to 1-pentene with peroxide initiators

AU Speier, John L.; Webster, James A.

CS Mellon Inst. Ind. Research, Pittsburgh, PA

SO Journal of Organic Chemistry (1956), 21, 1044-6

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

AB cf. C.A. 50, 14606f. A continuation study has been made of the addition of Cl₃SiH (I) to 1-pentene (II) in the presence of peroxide initiators in which certain factors influencing the addition have been noted. A series of expts. were carried out in which I, II, and tert-Bu perbenzoate were mixed and sealed into small Claisen flasks, after a period of heating the flasks opened, and contents distilled. To these flasks were also added miscellaneous components thought likely to have an effect on the yields. Silicone grease, H₂O, alc., Ni, Pb, Zn, air, N, or CO₂ had little or no effect. Fe and its salts were outstanding in preventing the formation of adduct. Sn was a promoter at temps. lower than those normally effective. Sn and its salts showed no catalytic activity alone, however, but presumably through some action on the peroxide acted as an effective promoter. Sn mixed with SnCl₄ caused the addition to become violent even at room temperature. Various Sn samples showed increasing activity with increasing amts. of impurities. Expts. using various initiators showed differences. Bz₂O₂ was very active and gave high peroxide efficiencies, but in certain mixts. tended to react so rapidly as to make control difficult. Other initiators employed were N,N'-azobisisobutyronitrile, tert-Bu peracetate, di-tert-Bu peroxide, Me Am ketone peroxide, and tert-Bu perbenzoate. Pentyltrichlorosilane (III), b₇₄₂ 171.0°, n_{25D} 1.4379, d₂₅ 1.128, was obtained from all expts. Methylation of III with excess MeMgBr in Et₂O gave 80% pentyltrimethylsilane (IV), b₇₄₃ 139.3°, n_{25D} 1.4069, d₂₅ 0.7271. IV was also prepared by adding a mixture of C₅H₁₁Cl and Me₃SiCl to molten Na in refluxing PhMe. Under the same conditions 2-pentene yielded a pentyltrichlorosilane, b. 165-7°, n_{25D} 1.4455, d₂₅ 1.145, quite different from IV.

=> s 15 and polymerization
336010 POLYMERIZATION

=> d 1-18 bib abs

L8 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:176652 CAPLUS

DN 134:366627

TI Insulated molecular wires: dendritic encapsulation of poly(triacetylene) oligomers, attempted dendritic stabilization of novel poly(pentaacetylene) oligomers, and an organometallic approach to dendritic rods

AU Schenning, Albertus P. H. J.; Arndt, Jan-Dirk; Ito, Masato; Stoddart, Alison; Schreiber, Martin; Siemsen, Peter; Martin, Rainer E.; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice; Gramlich, Volker; Diederich, Francois

CS Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.

SO Helvetica Chimica Acta (2001), 84(2), 296-334

CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta

DT Journal

LA English

OS CASREACT 134:366627

AB Multinanometer-long end-capped poly(triacetylene) (PTA) and poly(pentaacetylene) (PPA) oligomers with dendritic side chains were synthesized as insulated mol. wires. PTA oligomers with laterally appended Frechet-type dendrons of first to third generation were prepared by attaching the dendrons to an (E)-enediynes by a Mitsunobu reaction and subsequent Glaser-Hay oligomerization under end-capping conditions. Whereas first-generation oligomers up to the pentamer were isolated, for reasons of steric overcrowding, only oligomers up to the trimer were formed at the second-generation level, and only the end-capped monomer and dimer were isolated at the third-generation level. By repetitive sequences of hydrosilylation (with the Karstedt catalyst), followed by allylation or vinylation, a series of carbosilane dendrons were also prepared. Attachment of the second-generation wedge to (E)-enediynes, followed by deprotection and subsequent end-capping Hay oligomerization, provided PTA oligomers with lateral carbosilane dendrons. UV/VIS Studies demonstrated that the insulating dendritic layers did not alter the electronic characteristics of the PTA backbone, even at the higher-generation levels. Despite distortion from planarity due to the bulky dendritic wedges, no loss of π -electron conjugation along the PTA backbone was detected. A surprising (E) \rightarrow (Z) isomerization of the diethynylethene (DEE) core in the third generation derivative was observed, possibly photosensitized by the bulky Frechet-type dendritic wedge. Electrochem. investigations by steady-state voltammetry and cyclic voltammetry showed that the first reduction potential of the PTA oligomer with Frechet-type dendrons is shifted to more neg. values as the dendritic coverage increases. The first oligomers with a poly(pentaacetylene) backbone were obtained by oxidative Hay oligomerization under end-capping conditions. The synthesis of dendritic PPA oligomers by oxidative coupling of (E)-enetetrayne under end-capping conditions provided oligomers, which were formed as mixts. of stereoisomers due to unexpected thermal (E) \rightarrow (Z) isomerization. In another novel approach towards dendritic encapsulation of mol. wires with a Pt-bridged tetraethynylethene (TEE) oligomeric backbone, the trans-dichloroplatinum(II) complex with dendritic phosphane ligands was coupled under Hagihara conditions to mono-deprotected under formation of the extended monomer. Again, an unexpected thermal (E) \rightarrow (Z) isomerization, possibly induced by steric strain between TEE moieties and dendritic phosphane ligands in the unstable complex, led to isomeric mixture only.

RE.CNT 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:437042 CAPLUS

DN 133:177577
TI Synthesis of layered dendritic carbosilanes
AU Kim, C.; Choi, S. K.; Kim, B.
CS Department of Chemistry, Dong-A University, Pusan, 604-714, S. Korea
SO Polyhedron (2000), 19(9), 1031-1036
CODEN: PLYHDE; ISSN: 0277-5387

PB Elsevier Science Ltd.

DT Journal

LA English

AB Layered dendritic carbosilanes containing triple bonds on the peripheral layer, double bonds in the (n-1)th inner shell, and single bonds in the (n-2)th inner shell were prepared. The synthetic pathways used iterative hydrosilylation, alkenylation, and alkynylation. The fourth generation G4-E96PA is composed of two generations of propylene layers (G1 and G2) and one ethenyl layer in the inner shell (G3), and 96 ethynyl groups on the periphery (G4). The dendrimers are characterized by NMR, MALDI-TOF mass spectrometry, UV, IR, SEC and elemental anal.

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:306503 CAPLUS

DN 133:89822

TI Copper(I) Bromide/N-(n-Octyl)-2-pyridylmethanimine-Mediated Living-Radical Polymerization of Methyl Methacrylate Using Carbosilane Dendritic Initiators

AU Hovestad, Neldes J.; van Koten, Gerard; Bon, Stefan A. F.; Haddleton, David M.

CS Debye Institute Department of Metal-Mediated Synthesis, Utrecht University, Utrecht, 3584 CH, Neth.

SO Macromolecules (2000), 33(11), 4048-4052

CODEN: MAMOBX; ISSN: 0024-9297

PB American Chemical Society

DT Journal

LA English

AB The zeroth ($\text{Si}\{(\text{CH}_2)_3\text{SiMe}_2(\text{C}_6\text{H}_4\text{CH}_2\text{OC}(\text{O})\text{CMe}_2\text{Br})\}_4$), (2), and first ($\text{Si}\{(\text{CH}_2)_3\text{Si}((\text{CH}_2)_3\text{SiMe}_2(\text{C}_6\text{H}_4\text{CH}_2\text{OC}(\text{O})\text{CMe}_2\text{Br}))_3\}_4$), (3), generation of 2-bromoisobutyryl functionalized carbosilane dendrimers have been successfully applied as initiators for the copper(I) bromide/N-(n-octyl)-2-pyridylmethanimine-mediated living-radical polymerization of Me methacrylate. The overall rate of polymerization are comparable for the two dendritic initiators studied, 2 ($3.4 \times 10^{-5} \text{ mol L}^{-1} \text{ s}^{-1}$) and 3 ($4.8 \times 10^{-5} \text{ mol L}^{-1} \text{ s}^{-1}$) with the benzylic model compound $\text{C}_6\text{H}_5\text{CH}_2\text{OC}(\text{O})\text{CMe}_2\text{Br}$ (1) showing a lower rate of polymerization for both dendritic initiators, ($7.3 \times 10^{-5} \text{ mol L}^{-1} \text{ s}^{-1}$) where $[\text{initiator sites}] = 1.87 \times 10^{-2} \text{ mol L}^{-1}$. We postulate that this is caused by initial intramol. termination. The mol. weight distribution is less than 1.3 after 3 h reaction time. Initiator 3, however, produces star-star coupling throughout the polymerization. When the dendritic periphery is partially functionalized (statistically two and six arms of the first generation dendrimer, resp., 4 and 5) the control of the mol. weight distribution was lost ($\text{PDI} > 3$) for 4 as a result of too low of a value for $[\text{initiator site}]$, i.e., $3.12 \times 10^{-3} \text{ mol L}^{-1}$.

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:305017 CAPLUS

DN 133:105421

TI Modular Construction of Dendritic Carbosilanes. Organization of Dendrimer Connectivity around Bifunctional Precursors That Are Adapted for Sequential Convergent and Divergent Propagative Steps

AU Casado, Miguel Angel; Stobart, Stephen R.

CS Department of Chemistry, University of Victoria, BC, V8W 2Y2, Can.

SO Organic Letters (2000), 2(11), 1549-1552
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 AB Regiospecific hydrosilylation of 1-bromo-4-(prop-2-enyl)benzene offers an efficient route to mol. building block precursors that can accommodate sequential divergent and convergent steps for dendritic extension, establishing a modular methodol. for assembly and organization of connectivity used for synthesis of modified carbosilane dendrimers including $\text{Si}[\text{CH}_2\text{CH}_2\text{CH}_2\text{SiMe}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{-p-C}_6\text{H}_4\text{-p-C}_6\text{H}_4\text{CH}_2\text{CH}_2\text{SiMe}[\text{CH}_2\text{CH}_2\text{CH}_2\text{SiMe}[\text{CH}_2\text{CH}_2\text{CH}_2\text{SiMe}(\text{CH}_2\text{CH}=\text{CH}_2)_2]_2]_2]_4$.
 RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1999:558865 CAPLUS
 DN 132:152194
 TI Atom transfer polymerization of methyl methacrylate initiated by carbosilane dendritic species
 AU Hovestad, Neldes J.; Jastrzebski, Johann T. B. H.; Van Koten, Gerard; Bon, Stefan A. F.; Waterson, Carl; Haddleton, David M.
 CS Debye Institute, Department of Metal-Mediated Synthesis, Utrecht University, Utrecht, 3584 CH, Neth.
 SO Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1999), 40(2), 393-394
 CODEN: ACPPAY; ISSN: 0032-3934
 PB American Chemical Society, Division of Polymer Chemistry
 DT Journal
 LA English
 AB Zero- and first-generation carbosilane dendrimers were functionalized with a tertiary bromide species to be used as initiating compds. in atom transfer polymerization A kinetic study showed that atom transfer polymerization of Me methacrylate mediated by copper bromide and Schiff's base ligands was possible and produced star polymers with narrow mol. weight distributions.
 RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1999:334360 CAPLUS
 DN 131:116617
 TI Synthesis of carbosilane liquid-crystalline dendrimers of the first-fifth generations containing terminal cyanobiphenyl groups
 AU Ponomarenko, S. A.; Rebrov, E. A.; Boiko, N. I.; Muzafarov, A. M.; Shibaev, V. P.
 CS Department of Chemistry, Moscow State University, Moscow, 119899, Russia
 SO Vysokomolekulyarnye Soedineniya, Seriya A i Seriya B (1998), 40(8), 1253-1265
 CODEN: VSSBEE; ISSN: 1023-3091
 PB MAIK Nauka
 DT Journal
 LA Russian
 AB Carbosilane LC dendrimers of the first-fifth generations containing 8, 16, 32, 64, and 128 cyanobiphenyl terminal mesogenic groups, resp., were synthesized according to the divergent scheme. The synthesis of both the starting carbosilane dendrimers with the terminal allylic groups and the resulting LC compounds is described. The synthetic method is based on a Grignard reaction-hydrosilylation cycle, and silane bearing cyanobiphenyl groups linked via a spacer of 1 I methylene groups is added at the last stage of synthesis. The structure and the individuality of all the new dendrimers were established by NMR spectroscopy and gel-permeation chromatog. All the resulting dendrimers display LC mesophase in a wide temperature range.

L8 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1998:699732 CAPLUS
 DN 130:38734
 TI Termination of carbosilane dendrimers based on hexaallylethylenedisilane as core molecule
 AU Kim, Chungkyun; Jeong, Younsook
 CS Department of Chemistry, Dong-A University, Pusan, 604-714, S. Korea
 SO Main Group Metal Chemistry (1998), 21(10), 593-599
 CODEN: MGMCE8; ISSN: 0792-1241
 PB Freund Publishing House Ltd.
 DT Journal
 LA English
 AB Dendritic carbosilanes based on hexaallylethylenedisilane ((CH₂=CHCH₂)₃SiCH₂)₂ as a core mol. and allyl-groups as growth generation were prepared. The reaction path of the repetitive hydrosilation-alkenylation cycles is revealed by NMR spectroscopy. Each of the 2 steps in the hydrosilation-alkenylation process provided quant. yields of pure dendrimers. The termination of the dichloromethylsilyl-group contained third generation (G3P with Cl₂MeSi-groups) and chlorodimethylsilyl-group contained fourth generation (G4P with ClMe₂Si-groups) with allylmagnesium bromide, p-bromophenol, p-phenylphenol, LiAlH₄, and Li phenylacetylide were performed. All of the terminated dendrimers can be obtained as pure substances after simple chromatog. purification. They are characterized by spectroscopic analyses (NMR, MALDI mass, UV and IR) as well as elemental analyses.

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1997:777187 CAPLUS
 DN 128:75714
 TI Synthesis of polyolithium derivatives of carbosilane dendrimers
 AU Vasilenko, N. G.; Getmanova, E. V.; Myakushev, V. D.; Rebrov, E. A.; Moller, M.; Muzafarov, A. M.
 CS Institute of Synthetic Polymeric Materials, Russian Academy of Sciences, Moscow, 117393, Russia
 SO Vysokomolekulyarnye Soedineniya, Seriya A i Seriya B (1997), 39(9), 1449-1455
 CODEN: VSSBEE; ISSN: 1023-3091
 PB MAIK Nauka
 DT Journal
 LA Russian
 AB Methylbidecylsilyl-derivs. of polyallylcarbosilane dendrimers of the second and third generations bearing unsatd. groups in the inner sphere were synthesized. Organolithium compds. containing 8 and 16 lithium atoms were synthesized on their basis. The arrangement of lithium atoms in the inner sphere of a dendrimer prevents their intermol. aggregation. The synthesized compds. are new polyfunctional initiators of anionic polymerization, which show good solubility in organic solvents and which have reaction centers of equal activity. Using polymerization of hexamethylcyclotrisiloxane as an example, it was shown that these initiators are highly efficient catalysts in the synthesis of star-shaped polymers with the active functional groups at the ends of the arms.

L8 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1997:483983 CAPLUS
 DN 127:176800
 TI Dendrimers Containing Organometallic Moieties Electronically Communicated
 AU Cuadrado, Isabel; Casado, Carmen M.; Alonso, Beatriz; Moran, Moises; Losada, Jose; Belsky, Vitaly
 CS Departamento de Quimica Inorganica, Universidad Autonoma de Madrid,

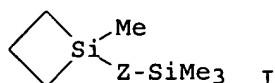
Madrid, 28049-, Spain
 SO Journal of the American Chemical Society (1997), 119(32),
 7613-7614
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 AB First and second generations of dendrimers and dendrons possessing
 ferrocenyl units electronically communicated have been constructed. The
 synthesis has been achieved following a convergent approach, starting from
 a vinyl-functionalized silicon-bridged biferrocene as a dendron, which has
 been characterized by X-ray crystallog. The novel dendritic mols. containing
 up to sixteen ferrocenyl moieties at the surface have been structurally
 characterized by ¹H, and ¹³C NMR, IR spectroscopy, elemental anal., and
 mass spectrometry. Solution electrochem. studies showed significant
 electronic interactions between peripheral ferrocenyl moieties which are
 linked by a bridging silicon atom. Electrodes modified with electroactive
 films of dendrimers carrying interacting ferrocenyl units, have been
 prepared
 RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1997:184981 CAPLUS
 DN 126:238723
 TI Chemistry of silane arborols. VII. Preparation of carbosilane dendrimers
 based on siloxane tetramer: silane arborols
 AU Kim, Chungkyun; An, Kyungmi
 CS Department Chemistry, Dong-A University, Pusan, 604-714, S. Korea
 SO Bulletin of the Korean Chemical Society (1997), 18(2), 164-170
 CODEN: BKCSDE; ISSN: 0253-2964
 PB Korean Chemical Society
 DT Journal
 LA English
 AB Via hydrosilylation-alkenylation approach using hydrosilanes (HSiMeCl₂ and
 HSiCl₃) and allylmagnesium bromide with siloxane tetramer (MeCH₂=CHSiO)₄
 as core mol., noble carbosilane dendrimers with 12, 24, 48 and 96 allylic
 end groups were prepared. The reaction path of the repetitive alkenylation
 and hydrosilylation was monitored by means of NMR spectroscopic
 measurements. Every step for the formation of dendrimer provided almost
 quant. yields as pure dendrimers. Based on the observation of UV
 spectroscopic measurements of Ga (n-1-4) mols. containing allylic end groups,
 the maximal molal absorption coeffs. (ε_{max}) at λ_{max} and the
 number of double bonds proved an exponentially increased correlation.
 RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1994:558309 CAPLUS
 DN 121:158309
 TI Fluorescently labeled polyallylcarbosilane dendrimers
 AU Krasovskii, V. G.; Sadvskii, N. A.; Gorbatshevich, O. B.; Muzafarov, A.
 M.; Myakushev, V. D.; Il'ina, M. N.; Dubovik, I. I.; Strelkova, T. V.;
 Papkov, V. S.
 CS Inst. Synthetic Polymeric Maters., Moscow, 117393, Russia
 SO Vysokomolekulyarnye Soedineniya, Seriya A i Seriya B (1994),
 36(4), 714-20
 CODEN: VSSBEE; ISSN: 1023-3091
 DT Journal
 LA Russian
 AB Polyallylcarbosilane dendrimers labeled by a fluorescent probe (pyrenyl)
 on the central silicon atom were first prepared. The compds. obtained were
 studied by NMR and UV spectroscopies, gel permeation chromatog. (GPC), and
 differential scanning calorimetry (DSC) and their fluorescence spectra

were also recorded. The possibility to study the intramol. structure of dendritic macromols. is demonstrated.

L8 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1992:256191 CAPLUS
DN 116:256191
TI Synthesis of polysiltrimethylenes with trimethylsilyl groups in the branch of main chain
AU Finkel'shtein, E. Sh.; Ushakov, N. V.; Pritula, N. A.; Andreev, E. A.; Plate, N. A.
CS A. V. Topchiev Inst. Pet. Chem. Synth., Moscow, 117912, USSR
SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1992), (1), 223-5
CODEN: IASKA6; ISSN: 0002-3353
DT Journal
LA Russian
GI



AB Thermally initiated or Pd catalyst-initiated polymerization of 1-silacyclobutanes
(I) [Z is CH₂, (CH₂)₃, or p-C₆H₄] gave soluble high-mol.-weight polycarbosilanes
with Me₃Si groups attached to the main chain via various bridges.

L8 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1980:568679 CAPLUS
DN 93:168679
TI Role of the stability of lithium poly(vinyltrimethylsilane) in the anionic polymerization of vinyltrimethylsilane
AU Bryantseva, I. S.; Khotimskii, V. S.; Durgar'yan, S. G.; Nametkin, N. S.
CS Inst. Neftekhim. Sint. im. Topchieva, Moscow, USSR
SO Doklady Akademii Nauk SSSR (1980), 251(4), 878-82 [Chem.]
CODEN: DANKAS; ISSN: 0002-3264
DT Journal
LA Russian

AB An investigation of model reactions indicated that polymerization of CH₂:CHSiMe₃
(I) [754-05-2] initiated by sec-BuLi [598-30-1] is accompanied by spontaneous cleavage of the C-Li bonds in the growing macromols., producing LiH. At >100° LiH initiates the polymerization of I, but at <100° the elimination of LiH reduces the concentration of living chains. The model reactions included decomposition of Li poly(trimethylvinylsilane) [75026-46-9] (mol. weight 6800) in hexane at 25-120° to LiH and the corresponding olefin, initiation of the polymerization of I by LiH, and anal.
of
products formed in the reaction of sec-BuLi with I under selected conditions.

L8 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1979:204178 CAPLUS
DN 90:204178
TI Oligomerization of vinyl- and ethynyltrimethylsilanes
AU Yur'ev, V. P.; Gailiunas, G.; Yusupova, F. G.; Nuritdinova, G. V.; Monakhova, E. S.; Tolstikov, G. A.
CS Inst. Chem., Ufa, USSR

SO Journal of Organometallic Chemistry (1979), 169(1), 19-24
 CODEN: JORCAI; ISSN: 0022-328X

DT Journal
 LA English
 OS CASREACT 90:204178

AB Oligomerization of vinyl- and ethynyltrimethylsilanes in the presence of homogeneous Ni, Co and Ti catalytic systems were studied. Vinyltrimethylsilane forms linear dimeric products, 1,4-bis(trimethylsilyl)butenes. Using the Ti catalytic system, in addition to butenyldisilane, a branched dimeric product, 1,3-bis(trimethylsilyl)-3-methylprop-1-ene, and a linear trimer 1,3,6-tris(trimethylsilyl)hex-3-ene are formed. Ethynyltrimethylsilane, in the presence of the Ni catalytic system, is converted into a linear dimer, 1,4-bis(trimethylsilyl)but-3-en-1-yne, and linear trimer, 1,4,6-tris(trimethylsilyl)hex-3,5-dien-1-yne.

L8 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1970:435806 CAPLUS
 DN 73:35806
 TI Synthesis of polysilylureas and polysilylureilenes
 AU Gol'din, G. S.; Tsiomo, S. N.; Shchekina, T. V.; Kozyukov, V. P.
 CS USSR
 SO Vysokomolekulyarnye Soedineniya, Seriya B: Kratkie Soobshcheniya (1970), 12(4), 307-9
 CODEN: VYSBAI; ISSN: 0507-5483

DT Journal
 LA Russian
 GI For diagram(s), see printed CA Issue.

AB Oligomeric poly(silylureas) [I, R = O, CH₂, (CH₂)₂, or (CH₂)₃] were prepared by a reaction of bis[(γ-isocyanatopropyl)dimethylsilyl]-alkanes (II) or 1,3-bis(γ-isocyanatopropyl)-1,1,3,3-tetramethyldisiloxane (III) with MeNH(CH₂)₂NHMe. Reaction of N₂H₄ or PhNHNH₂ with II or III gave poly(silylureylenes) [IV, R = O or (CH₂)₃], almost insol. in organic solvents. The structure of the polymers was determined by ir spectroscopy and elemental anal.

L8 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1965:446342 CAPLUS
 DN 63:46342
 OREF 63:8393g-h,8394a

TI Platinum-catalyzed reactions of silacyclobutanes and 1,3-disilacyclobutanes

AU Weyenberg, Donald R.; Nelson, Lee E.
 CS Dow Corning Corp., Midland, MI
 SO Journal of Organic Chemistry (1965), 30(8), 2618-21
 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal
 LA English

AB Platinum has been found to be a catalyst for the ring-opening polymerization of silacyclobutanes (I) and 1,1,3,3-tetramethyl-1,3-disilacyclobutane (II). The structures of the polymers were shown to be [R₂Si(CH₂)₃]_x and [Me₂SiCH₂]_x by comparison of their ¹H N.M.R. and infrared spectra to model structures. Platinum also catalyzed the interaction of silicon hydrides (R'₃SiH) with I and II to give telomeric structures, R'₃Si[(CH₂)₂SiR₂]_xH and R'₃Si[CH₂SiMe₂]_{2x}H. Studies with phenyldimethylsilane-d show that this reaction involves exchange of the silicon-hydrogen bond of the hydride and the ring silicon-carbon bond of I and is thus the first example of a platinum-catalyzed exchange of alkyl and hydrogen on silicon.

L8 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 1964:440520 CAPLUS
 DN 61:40520
 OREF 61:7039e-f

TI Telomerization of silicacyclobutanes

AU Nametkin, N. S.; Vdovin, V. M.; Grinberg, P. L.
CS Inst. Petrochem. Synth., Moscow
SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1964), (6),
1133-4
CODEN: IASKA6; ISSN: 0002-3353
DT Journal
LA Unavailable
AB Refluxing R_3SiH with 1,1-dialkyl-1-silacyclobutanes with or without added
Pt catalyst several hrs. resulted in formation of $R_3Si(CH_2CH_2CH_2SiR'_2)_nH$.
With $R = Et$ and $R' = Me$, the following telomers were isolated (n shown):
1, b3 63-5°, n20D 1.4452, d20 0.8033; 2, b1 116-18°, 1.4535,
0.8236. Higher telomers were also formed. The reaction was also
applicable to disilacyclobutanes.

L8 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1958:10900 CAPLUS
DN 52:10900

OREF 52:1917e-f

TI The mode of peroxide-catalyzed polymerization of
vinyl-triethoxysilane

AU Mixer, R. Y.; Bailey, D. L.
CS Linde Air Products. Co., Tonawanda, NY
SO Journal of Polymer Science (1955), 18, 573-82
CODEN: JPSCAU; ISSN: 0022-3832

DT Journal

LA Unavailable

AB It has been qualitatively demonstrated that vinyltriethoxysilane, b30
70°, n25D 1.3966, d25 0.9036, MRD 50.66, is polymerized by a free
radical process to clear, colorless viscous liquid polymer of low mol. weight
The low mol. weight is the result of chain transfer with polymer and monomer.
This chain transfer involves the abstraction of the α -H of an
ethoxysilyl group of either the polymer or the monomer. The ratio of
chain transfer with polymer to that with monomer for high conversion is at
least 4.5.